



chain nodes :  
 7 9 12 13 15 16 17 19  
 ring nodes :  
 1 2 3 4 5 6  
 chain bonds :  
 1-9 4-7 12-13 15-16 17-19  
 ring bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6  
 exact/norm bonds :  
 1-9 4-7 12-13 15-16 17-19  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6

G3 : X, CH2, CF3, CCl3, CO2H, CN, SO3H, CHO, C(O)CH3

G4 : X, Ak, MeO, EtO, n-PrO, i-PrO, n-BuO, i-BuO, s-BuO, t-BuO, NO2

G5 : H, NO2, X, Cb, Cy, Hy, Ak

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 12:CLASS 13:CLASS 15:CLASS  
 16:CLASS 17:CLASS 19:CLASS